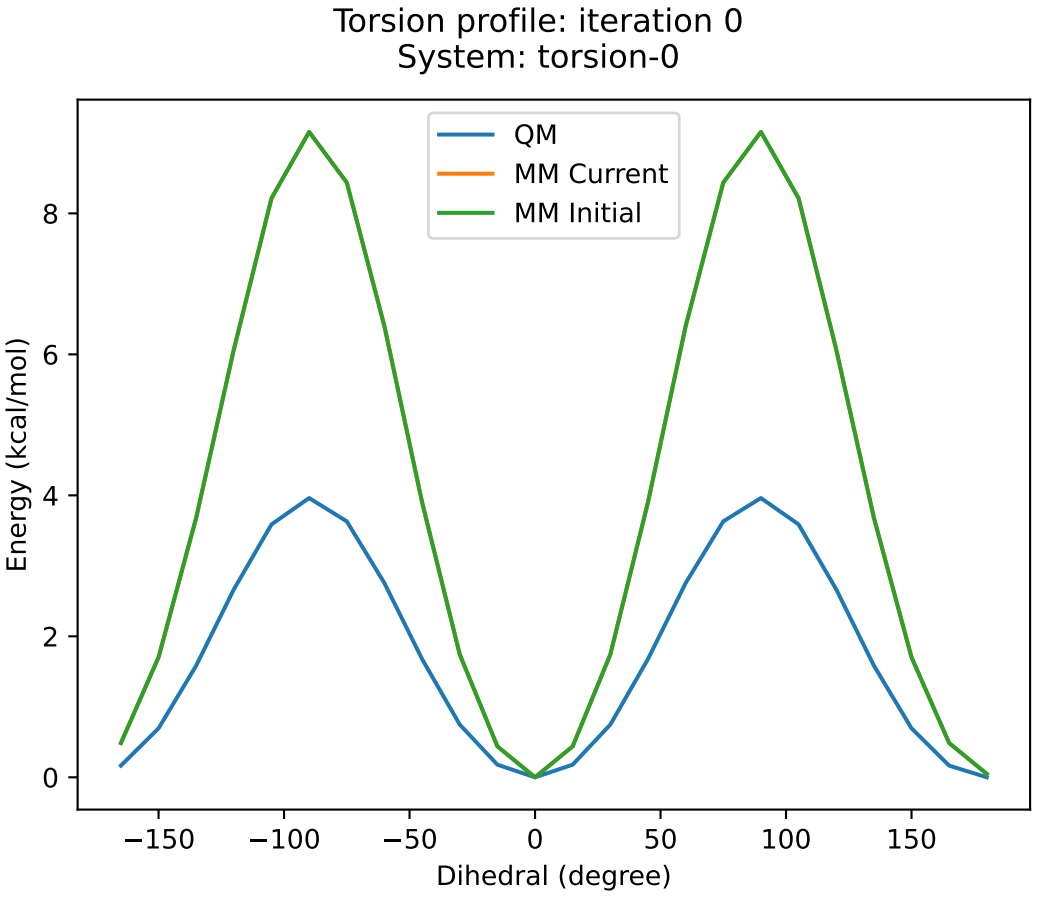
Torsion profile: iteration 0
System: torsion-0
QM
MM Current
MM Initial
Energy (kcal/mol)
0
2
4
6
8
−150
−100
−50
0
50
100
150
Dihedral (degree)